

WHAT IS CLAIMED IS:

1. A method for the automated production and iterative automated optimization of a substance library having at least two substances or at least one reaction parameter relating to a performance characteristic of the substance library, the method comprising the steps of:

- a) defining at least one production parameter and at least one test parameter;
- b) automated preparation of the substance library by producing at least two substances on the basis of the at least one production parameter;
- c) automated testing of the at least two substances of the substance library with respect to at least one performance characteristic on the basis of the at least one test parameter;
- d) evaluating the test using electronic data analysis; and
- e) varying the at least one production parameter and/or the at least one test parameter for optimizing the performance characteristics, to perform single or repeated iterations of steps b) to e) or c) to e);

wherein the steps b) to e) are carried out as an integrated automated process.

2. The method according to claim 1, wherein the results of the tests in step c) are stored in a database together with the associated at least one production parameter and/or test parameter.

3. The method according to claim 2, wherein the results are stored using a system time, the system location of at least one

substance in the substance library and/or the substance identification as assignment criterion.

4. The method according to claim 1, wherein one or more effects of individual production parameters and test parameters on performance characteristics is determined by data analysis.

5. The method according to claim 2, wherein one or more effects of individual production parameters and test parameters on performance characteristics is determined by data analysis.

6. The method according to claim 3, wherein one or more effects of individual production parameters and test parameters on performance characteristics is determined by data analysis.

7. The method according to claim 1, wherein the data analysis comprises using classical statistical methods, regression methods, linear or nonlinear regression, data mining methods, neural networks or evolutionary methods.

8. The method according to claim 4, wherein parameters determined by data analysis as having a negligible effect on the performance characteristics are either kept constant or are not considered in subsequent iterations in step d).

9. The method according to claim 7, wherein parameters determined by data analysis as having a negligible effect on the performance characteristics are either kept constant in subsequent iterations or are not considered in step d).

10. The method according to claim 1, wherein the at least two substances comprise either molecular substances, non-molecular substances, formulations, materials, or mixtures of two or more thereof.

11. The method according to claim 10, wherein the at least two substances of the substance library are selected from the group consisting of heterogeneous or heterogenized catalysts, luminophores, electrooptical, superconducting or magnetic substances, or mixtures of two or more thereof.

12. The method according to claim 10, wherein the at least two substances of the substance library are selected from the group consisting of intermetallic compounds, oxides, oxide mixtures, mixed oxides, ionic or covalent compounds of metals and/or nonmetals, metal alloys, ceramics, organometallic compounds and composite materials, dielectrics, thermoelectrics, magnetoresistive and magnetooptical materials, organic compounds, enzymes, active pharmaceutical compounds, substances for foodstuffs and food supplements, feedstuffs and feed supplements and cosmetics and mixtures of two or more thereof.

13. The method according to claim 10, wherein the performance characteristics comprise activity and selectivity in one or more chemical reactions catalysed by at least one catalyst.

14. The method according to claim 11, wherein the performance characteristics comprise activity and selectivity in one or more chemical reactions catalysed by at least one catalyst.

Figure 1

Diagram illustrating the experimental setup for measuring the effect of temperature on the rate of polymerization. The setup includes a reaction vessel containing monomer and initiator, connected to a gas-liquid separator, which is further connected to a gas flow meter and a pressure transducer. The reaction vessel is submerged in a water bath maintained at a constant temperature.

Figure 1

Diagram illustrating the experimental setup for measuring the effect of temperature on the rate of polymerization. The setup includes a reaction vessel (A) connected to a gas-liquid separator (B), which is further connected to a gas flow meter (C). The reaction mixture is heated by a jacket (D) containing a heating medium (E). The temperature of the reaction mixture is monitored by a thermometer (F). The gas flow rate is measured by a gas flow meter (G).

E

Figure 1

Diagram illustrating the experimental setup for measuring the effect of temperature on the rate of reaction between hydrogen peroxide and potassium iodide.

The diagram shows a test tube containing a mixture of hydrogen peroxide (H_2O_2) and potassium iodide (KI). The test tube is placed in a water bath maintained at a constant temperature ($T^\circ C$). A gas syringe is connected to the test tube to measure the volume of oxygen gas (O_2) produced over time. The reaction is initiated by adding a catalyst (e.g., manganese(IV) oxide, MnO_2).

The diagram also includes a graph showing the volume of oxygen gas produced versus time. The curve starts at the origin and rises steeply, indicating a rapid initial rate of reaction, before leveling off as the reaction proceeds towards completion.

Figure 1

Diagram illustrating the experimental setup for measuring the effect of temperature on the rate of polymerization. The setup includes a reaction vessel containing monomer and initiator, connected to a gas-liquid separator, which is further connected to a gas flow meter and a pressure transducer. The reaction vessel is heated by a jacketed coil through which a heating fluid circulates. The gas flow meter measures the volume of gas evolved, and the pressure transducer monitors the system pressure.

[illegible]

a test device that tests the at least two substances of the substance library with respect to at least one performance characteristic on the basis of the at least one test parameter;

a data analysis system for evaluating the tests;

a device for varying the at least one production parameter and/or test parameter for optimising the performance characteristics, and

control means for integrated and automated control of the defining means, the preparation means, the test device, the data analysis system, and the device.

20. The apparatus according to claim 19 further comprising storage means for storing test results in a database associated with at least one production parameter and/or test parameter and/or system time or absolute position of the tested substance.

21. Substrate comprising at least one substance library comprising at least two substances, wherein the substance library is obtainable by a method for the automated production and iterative automated optimization of a substance library and/or at least one reaction parameter, the method comprising the steps:

a) defining at least one production parameter and at least one test parameter;

b) automated preparation of a substance library by producing at least two substances on the basis of the at least one production parameter;

c) automated testing of the at least two substances of the substance library with respect to at least one desired useful property on the basis of the at least one test parameter;

d) evaluating the test using electronic data analysis; and

e) varying the at least one production parameter and/or the at least one test parameter for optimizing the desired useful properties, to perform single or repeated iterations of steps b) to e) or c) to e), wherein the steps b) to e) are carried out as an integrated automated process.

22. A computer readable data storage medium having computer program code recorded thereon executable by a computer, the computer program code comprising:

a first program code for defining at least one production parameter and at least one test parameter;

a second program code for automated preparation of a substance library by producing at least two substances on the basis of the at least one production parameter;

a third program code for automated testing of the at least two substances of the substance library with respect to at least one performance characteristic on the basis of the at least one test parameter;

a fourth program code that evaluates the test using data analysis;

a fifth program code that varies the at least one production parameter and/or the at least one test parameter for optimizing the test characteristics and to perform single or repeated iterations of the first to fourth program codes; and

a control program code that controls execution of the first to fifth program codes as an automated and integrated process.

23. The computer readable data storage medium according to claim 22, further comprising:

24. The computer readable data storage medium according to claim 22, wherein the fourth program code evaluates effects of individual production parameters and test parameters on performance characteristics.

25. The computer readable data storage medium according to claim 22, wherein the data analysis comprises classical statistical methods, regression methods, linear or nonlinear regression, data mining methods, neural networks, or evolutionary methods.

26. The computer readable data storage medium according to claim 22, wherein parameters determined by the fourth program code as having a negligible effect on the performance characteristics is either kept constant or not considered in subsequent iterations by the fifth program code.

27. The computer readable data storage medium according to claim 22, wherein the at least two substances comprise either molecular substances, non-molecular substances, formulations, materials, or mixtures of two or more thereof.

28. The computer readable data storage medium according to claim 22, wherein the at least two substances of the substance library are selected from heterogeneous or heterogenized catalysts, luminophores, electrooptical, superconducting or magnetic substances, or mixtures of two or more thereof.

29. The computer readable data storage medium according to claim 22, wherein the at least two substances of the substance library are selected from intermetallic compounds, oxides, oxide mixtures, mixed oxides, ionic or covalent compounds of metals and/or nonmetals, metal alloys, ceramics, organometallic compounds and composite materials, dielectrics, thermoelectrics, magnetoresistive and magneto-optical materials, organic compounds, enzymes, active pharmaceutical compounds, substances for foodstuffs and food supplements, feedstuffs and feed supplements and cosmetics and mixtures of two or more thereof.

30. The computer readable data storage medium according to claim 22, wherein the performance characteristics comprise activity and selectivity in one or more chemical reactions catalysed by at least one catalyst.

31. The computer readable data storage medium according to claim 22, wherein the test parameters comprise reactor type, operating temperature of the at least one catalyst and/or of the starting material fluid and the pressure and/or the composition of the starting material fluid and/or residence time and/or space velocity.

32. The computer readable data storage medium according to claim 22, wherein the substance library is either arranged linearly or in a multidimensional matrix.